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JACKKNIFE, RIDGE AND ORDINARY LEAST SQUARES ESTIMATORS OF REGRE--ETC(U)

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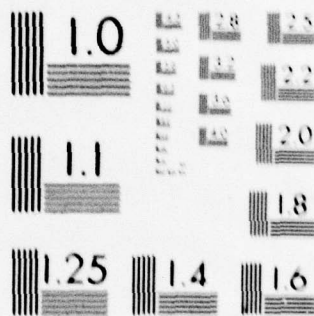
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Jackknife, Ridge and Ordinary Least Squares

Estimators of Regression Parameters:

A Monte Carlo Comparison

September, 1979

Michael K. Lindell

Battelle Human Affairs Research Centers
Seattle, Washington

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This study reports the results of a Monte Carlo evaluation of the small sample performance of ordinary least squares (OLS), ridge, and jackknife estimators of regression coefficients. The primary criteria of evaluation are the mean square error (MSE) of the regression coefficients and the size of the t-statistics associated with these coefficients. The conditions studied are derived from a design in which two factors are varied: the sample size to number of predictors (N/p) ratio and the metric quality of the data (dichotomous and polychotomous).

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Multicollinearity produces many problems in the analysis of data by multiple regression. One of the most common of these problems is the "bizarre" regression coefficients that are sometimes found. In some cases one or more of the standardized coefficients is greater than unity in absolute value. This is particularly unsettling when two items measuring the same underlying factor and having approximately equal correlations with the dependent variable are entered into an equation and one of the coefficients gets the "wrong sign." That is, the sign of the regression weight is the opposite of the sign of the correlation between that variable and the dependent variable.

A wide range of techniques have been developed to deal with problems such as this (see Dempster, Schatzoff and Wermuth, 1977, for a study of 57 varieties of estimators). Many of these, including variable selection and ridge regression, can be used to "shrink" the regression weights by ignoring certain aspects or reducing the influence of certain parts of the data matrix. The differences among the procedures arise from the ways in which they accomplish this function. Variable selection techniques, the most commonly recommended solution, reduce the effects of multicollinearity by deleting variables. Stepwise regression algorithms, for example, typically admit additional variables into a regression equation only if the multiple correlation of the additional variable with the already entered variables is acceptably low. This eliminates the problem of variables with "wrong signs" by deliberately causing the "wrong signs" to be replaced by zeros. That is, the equation associated with the simultaneous analysis of all of the variables,

$$[1] \quad Y = \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p + e$$

where \underline{Y} is the dependent measure, the $\underline{\beta}_i$ are the regression weights for the full set of p predictor variables, \underline{x}_i ; and \underline{e} is the error of prediction, is replaced by a restricted regression equation,

$$[2] \quad Y = \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_\ell x_\ell (+ 0x_{\ell+1} + \dots + 0x_p) + e$$

where the zeros before the variables within the parentheses denote that by deleting these variables, they have implicitly received a weight of zero in the regression equation.

A recently developed alternative to variable selection is ridge regression (Hoerl and Kennard, 1970, a, b). Although stepwise regression differs from ordinary least squares (OLS) in the way that the equations are specified, the difference between ridge regression and OLS is in the computation of the regression weights. OLS estimates of the regression weights are derived from the formula,

$$[3] \quad \underline{\beta} = \underline{R}^{-1} \underline{r}$$

where $\underline{\beta}$ is a vector of standardized regression weights, \underline{R} is the matrix of correlations among the predictor variables and \underline{r} is the vector of predictor-criterion correlations. Ridge coefficients are estimated from the equation,

$$[4] \quad \underline{\beta}^* = (\underline{R} + k\underline{I})^{-1} \underline{r}$$

where k is an arbitrary constant and \underline{I} is an identity matrix. In ridge regression, the elements on the diagonal of the predictor \underline{R} matrix are inflated so that they are large compared to the off-diagonal elements. As the size of the constant added to the diagonal increases, the

resulting estimates of the regression coefficients are "shrunk" toward zero. This shrinkage produces an estimator which is biased, but has less variance than the OLS estimator. The amount of bias increases with the magnitude of the constant, k .

Although the proper method of determining the value of the constant, k , has not been fully resolved, the subjective rules proposed by Hoerl and Kennard (1970, a, b; see also Price, 1977), have been supplanted by objective rules. Hoerl, Kennard and Baldwin (1975), for example, have recommended the use of the value,

$$[5] \quad k = p\sigma^2 / \sum \beta_i^2$$

where p is the number of predictor variables, σ^2 is the error variance and the β_i are, as before, the standardized regression coefficients.

In addition to concerns for reasonable looking regression weights, researchers are often interested in determining the statistical significance of the coefficients. This often involves the computation of standard errors and t -statistics for the individual coefficients. When high levels of multicollinearity are present, these statistics are also affected. Multicollinearity produces standard errors which are quite large and t -statistics which are small. This problem has caused some statisticians (see, for example, Press, 1975) to recommend that highly correlated variables be deleted and the regression equation reestimated. Note that this solution to the problem is an informal algorithm for backward deletion (Draper and Smith, 1966) which is another type of variable selection.

A ready tool which might be compared to OLS estimates of standard errors and t-statistics is the jackknife (Mosteller and Tukey, 1968). The jackknife procedure is a simple and widely applicable technique for computing robust estimates of many statistics and their associated standard errors. Its greatest value lies in situations in which there are no readily available techniques for calculating the standard error of a coefficient or when the analyst has reason to believe that conventional estimates of the standard error are inappropriate.

The key to the jackknife is the simple device of dividing a body of data into subsamples, creating "pseudovalue" by computing a weighted difference between the coefficients produced by analysis of the entire sample and the coefficients produced by analysis of each of the subsamples, and using the mean and standard deviation of the pseudovalue to generate estimates of the parameter and its standard error.

The first step of the jackknife requires that the body of data be divided into n subgroups of (approximately) equal size. Subsamples are formed by deleting each of the subgroups, in turn, from the body of data. Subsample 1 includes all but the first N/n observations, subsample 2, all but the next subgroup of N/n observations, and so on. In step two, a regression analysis is performed on the total sample and on each of the n subsamples. In step three these matrices of coefficients are converted to pseudovalue as computed by the following equation:

$$[6] \quad \theta(j) = (n - 1) \beta(j)$$

where $\underline{e}_{(j)}$ is the j^{th} vector of pseudovalues, \underline{n} is the number of subgroups, \underline{g} is the vector of regression coefficients derived from the analysis of the entire body of data, and $\underline{g}_{(j)}$ is the coefficient vector derived from the deletion of the j^{th} subsample. Step four reduces the obtained pseudovalues to means and standard deviations. The vector of means of the pseudovalues is the jackknifed estimate of the regression coefficient vector (\underline{g}_*) and each element of the vector of standard deviation of the pseudovalues divided by the square root of \underline{n} is an estimate of the standard error of the corresponding regression coefficient.

The purpose of the experiment reported in this paper was to compare OLS, ridge and jackknife estimates of regression coefficients under some conditions which reasonably approximate those existing in many situations of interest to psychologists. Two characteristics of data that are particularly important to study are the number of observations relative to the number of predictors ($\underline{N}/\underline{p}$ ratio) and the violation of the assumptions of the regression model. The $\underline{N}/\underline{p}$ ratio should be considered since low levels ($\underline{N}/\underline{p} \leq 5$) produce unstable estimates of regression weights which are very likely to be of the "bizarre" type discussed earlier. Violation of standard regression assumptions should be considered since failure of the errors to conform to the pattern, $E(\epsilon\epsilon') = \sigma^2 I$, can adversely affect the estimates of the standard errors of the regression coefficients.

METHOD

Violation of regression assumptions was produced by the use of discrete (dichotomous or polychotomous) rather than continuous scales of measurement on the dependent variable. The analysis of discrete dependent variables by OLS is, of course, strongly discouraged since, in this case, $E(\epsilon\epsilon') \neq \sigma^2 I$. This problem is particularly severe with dichotomous variables. Thus, the use of two different levels of metric quality provides a convenient means of assessing the sensitivity of OLS, ridge and jackknife to different levels of violation of regression assumptions. Three levels of N/p and two levels of metric quality (dichotomous and polychotomous) were used to form a factorial design.

Common to the resulting set of six conditions was a population predictor matrix, taken from Price (1977), shown in Table 1. The five predictor variables are highly collinear, as seen by the ratio of the largest eigenvalue to the smallest eigenvalue of the correlations matrix ($\lambda_1/\lambda_5 = 796$).

 Insert Table 1 About Here

Each of the replications of each of the six cells of the design matrix required the estimation of twelve regression equations--one OLS, one ridge and ten jackknife equations. In view of this substantial amount of computing, the study was limited to a single population regression equation. An equal weighted equation ($\underline{g}_i = .226, i = 1,5$) with an associated $\sigma_e^2 = 1 - R^2 = .20$, was chosen as a case which was particularly likely to challenge the utility of the Hoerl, et al.

(1975) bias coefficient estimator, \underline{k} . It can easily be seen that for this population regression equation, the values of \underline{k} estimated from equation [5] will equal (in the population), $(5)(.2)/.354 = 2.826$. Since estimated values of \underline{k} will consistently be greater than unity in the sample equations, equal weighted predictors will produce severely biased estimates of the \underline{g}_j .

The use of five predictor variables and three levels of $\underline{N/p}$ (5/1, 10/1 and 20/1) produced sample sizes of 25, 50 and 100. These can be considered to be marginally acceptable (5/1), recommended (10/1), and highly desirable (20/1) ratios of $\underline{N/p}$. The metric quality of the predictor variables was held constant (at five levels) across conditions. The dependent (criterion) variable set at either five levels (polychotomous) or two levels (dichotomous). Results for each of the six combinations of the two factors were based upon 500 replications of each of the three estimation techniques. That is, in each cell of the design matrix, 500 separate samples were generated.

The values of the predictor variables in each sample (the \underline{X} matrix) were computed by multiplying a matrix of independent standard (zero mean and unit variance) normally distributed pseudo-random numbers by the matrix of eigenvectors of the predictor R matrix. These random numbers were generated by subroutine GGNOR (IMSL, 1977). The value of the criterion variable was computed by post-multiplication of the sample \underline{X} matrix by the vector of standardized population regression coefficients and addition of an independent normally distributed pseudo-random error term ($N(0, \sqrt{2})$). Predictors and criterion were further transformed to the appropriate p-chotomous ($p = 5, 2$) variables by dividing the interval

between -3 and $+3$ standard deviations about the mean, $-3.0 \leq x \leq +3.0$, into p equal intervals. The discrete transformation process has a differential effect upon the moments of the sample distributions of the dichotomous and polychotomous dependent variables. As a result, "main effects" of metric quality are not only uninteresting (as they would be in any event) but ambiguous, as well. The nature of discrete transformation does not, however, affect the interpretation of interaction effects--such as method of analysis by metric quality or method of analysis by metric quality by sample size--which are discussed below.

Following generation of the sample values, the three regression procedures were executed. The standardized OLS coefficients were computed through solution of equation [3]. Standard errors of the regression coefficients were computed and t -ratios were formed. Ridge coefficients were computed through the use of equation [4] after the value of k had been estimated from the expression proposed by Hoerl, Kennard and Baldwin, contained in equation [5]. Standard errors of the ridge coefficients were derived from the square roots of diagonal elements of the matrix

$$[7] \quad V(\beta^*) = \sigma^2(R + kI)^{-1} R (R + kI)^{-1}$$

as shown by Marquart and Snee (1975, p. 6). Jackknifed regression coefficients and their standard errors were computed from the expressions

$$[8] \quad \beta_{*j} = \Sigma \theta_{(j)i} / n$$

$$[9] \quad \text{VAR}(\beta_{*1}) = \Sigma (\theta_{(j)i} - \beta_{*1})^2 / (n - 1)$$

At the end of the 500 replications, the accumulated data were converted to the statistics (a) mean squared error of the regression weights, (b) mean bias, (c) mean standard error of the regression weight, and (d) mean t-statistic. These criteria are defined by the expressions in Table 2.

 Insert Table 2 About Here

RESULTS

The data contained in Table 3 show that the MSE of OLS decreases with increasing sample size. This is as one would expect since MSE is composed of two components, bias and variance. Since OLS is unbiased and variance decreases with sample size, one should find this result. The pattern is repeated at both levels of metric quality although—again as one might expect—MSE is much higher for a dichotomous criterion variable than for a polychotomous criterion. The obtained levels of MSE for the jackknife coefficients are almost identical to those for OLS.

 Insert Table 3 About Here

Just the reverse pattern holds for the ridge estimator; the MSE increases with sample size. This interaction is a "crossover" or disordinal interaction. At 5/1 and 10/1, ridge has smaller MSE than OLS, but at 20/1, OLS has smaller MSE than ridge. The effect is even more pronounced for a dichotomous criterion than for a polychotomous

criterion. Ridge is much less sensitive to metric quality at small sample sizes ($N = 25$) than are OLS or jackknife.

Inspection of Table 4 suggests an explanation for this result. Although all OLS and jackknife estimates are slightly biased due to the attenuation caused by the discrete transformation, ridge coefficients are substantially biased. Moreover, this bias increases with increasing sample size.

Insert Table 4 About Here

Mean standard errors and mean t -statistics associated with each of the three estimation methods are displayed in Tables 5 and 6. Again, there are no appreciable differences between OLS and jackknifed estimates. The important contrast is between the estimated standard errors for ridge coefficients and those of OLS and jackknifed coefficients. The estimated standard errors of the ridge coefficients are not only consistently smaller, but the ratio $\overline{SE}(\beta) / \overline{SE}(\beta^*)$ gets larger with increasing sample size. Metric quality affects all three estimators. The dichotomous criterion produces higher estimated standard errors and lower t -statistics for all three estimators.

Insert Tables 5 and 6 About Here

DISCUSSION

The use of jackknife estimation is, under conditions like those studied here, clearly not warranted. Although jackknifed estimates of the \underline{g}_i are virtually identical to the OLS estimates, jackknifed coefficients require substantially more computational effort. The equivalence of jackknifed regression weights and OLS weights is no great surprise. As Wainer and Thissen (1977) have noted, studies of robust statistics have emphasized their usefulness in the presence of distributions which have longer tails than those of the normal distribution. The results obtained here are consistent with their remark that OLS will do quite well (compared to robust methods such as the jackknife) with short tailed distributions.

Since the estimated standard errors of the OLS and jackknifed coefficients are also the same, the mean \underline{t} -ratios are virtually identical. This is a substantial factor working against the jackknife. In the case of the \underline{t} -statistics, there is not only the additional computational burden, but the jackknifed \underline{t} -statistic is based upon fewer degrees of freedom ($\underline{n} - 1$ for the jackknife vs. $\underline{N} - \underline{p} - 1$ for OLS). The difference is substantial even at the lowest $\underline{N}/\underline{p}$ ratios studied here.

The superiority of the Hoerl, Kennard and Baldwin (HKB) ridge estimator over OLS at low levels of $\underline{N}/\underline{p}$ raises some interesting questions. Although the bias coefficients provided by equation [5] are intended to produce estimates which have smaller expected mean square error than OLS, they do not necessarily produce minimum mean squared error. The extreme level of bias produced in this situation leads one to wonder whether a less severely biased estimator might prove to be

superior to both OLS and the HKB estimator. In support of the HKB estimator, it should be noted that it can produce "reasonable looking" values for \underline{k} . For example, when applied to the Price (1977) data, including the initial OLS estimates of the $\underline{\beta}_i$ obtained by that author, equation [5] produces an estimate of \underline{k} that is virtually identical to the value that was derived subjectively from inspection of the ridge trace. Although the "true" model underlying the Price data is unknown, the initial OLS estimates of the regression coefficients varied considerably in magnitude. This, in turn, produced a large $\sum \underline{\beta}_i^2$ which resulted in a small ($\underline{k} = .06$) value of the bias coefficient. Whether or not the HKB estimator can be improved upon, the fact the choice between OLS and ridge regression is affected by the $\underline{N/p}$ ratio suggests that the importance of this factor, hitherto ignored in Monte Carlo studies of ridge regression, ought to be noted.

This conclusion may appear to be inconsistent with that of McDonald and Galarneau who stated that the performance of ridge estimators "depends on the variance of the random error, the correlations among the explanatory variables and the unknown coefficients vector" (1975, p. 416). However, the $\underline{N/p}$ ratio and the metric quality of the variables both act together with the true error variance to influence the estimated variance of the random error. They also act together with the correlations among the explanatory variables and the unknown coefficient vector to influence the OLS estimates of the regression coefficients. Since both the estimated variance of the random error and the estimated OLS regression coefficient vector are used to calculate the proper amount

of bias, k , to introduce into the ridge estimator, there is no real conflict between the results of this study and the conclusions drawn from prior studies of ridge regression.

That the standard errors of these ridge coefficients are substantially smaller than the corresponding OLS estimates and the t -statistics are correspondingly larger is also an interesting finding. To date, there has been no indication that these t -statistics are actually distributed as Student's t , and if so, with what number of degrees of freedom. The data shown in Table 6 suggest that an investigator who used the ridge estimates of the t -statistics as a rough indicator of statistical significance would be quite likely to reject the null hypothesis, $\beta_i = 0$. Such a procedure would, however, also lead one to reject a specific alternative hypothesis of $\beta_i = .226$, the population regression coefficients for this data set. To argue that specific alternative hypotheses are virtually nonexistent, though true, seems to beg the issue. A more satisfactory resolution to the problem may be to assert that bias in regression weights is a relatively unimportant consideration. What does make a difference to many, if not most investigators, is that the ratios of the weights be accurately determined. Put otherwise, one wants the orientation of the obtained weight vector in the parameter space to be close to that of the true regression vector. Estimates which are proportional to the true weights would, by this criterion, be equivalent. It seems reasonable that shrunken estimators such as ridge would be more likely than OLS to satisfy this proportionality criterion. The nature of the types of conditions under which they would do so remains to be determined.

FOOTNOTES

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TABLE 1

Zero-Order Correlations

x_1	x_2	x_3	x_4	x_5
1.000	.597	.669	.188	.867
	1.000	.640	.116	.819
		1.000	.377	.906
			1.000	.207
				1.000

$$\lambda_1/\lambda_5 = .796$$

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TABLE 2

<u>Criterion</u>	<u>Expression</u>			
Mean squared error	$\frac{1}{2500}$	$\sum_{\ell=1}^{500}$	$\sum_{i=1}^5$	$(\beta_{i\ell} - \hat{\beta}_{i\ell})^2$
Bias	$\frac{1}{2500}$	$\sum_{\ell=1}^{500}$	$\sum_{i=1}^5$	$(\beta_{i\ell} - \hat{\beta}_{i\ell})$
Mean standard error	$\frac{1}{2500}$	$\sum_{\ell=1}^{500}$	$\sum_{i=1}^5$	$SE(\hat{\beta}_{i\ell})$
Mean <u>t</u> -statistic	$\frac{1}{2500}$	$\sum_{\ell=1}^{500}$	$\sum_{i=1}^5$	$t_{\hat{\beta}_{i\ell}}$

TABLE 3

Mean Squared Error of Coefficients

Sample Size	Metric Quality of Criterion					
	Dichotomous			Polychotomous (5)		
	OLS	Ridge	Jackknife	OLS	Ridge	Jackknife
25	.607	.111	.638	.333	.080	.354
50	.262	.131	.266	.135	.092	.139
100	.125	.149	.125	.066	.101	.067

TABLE 4

Bias of Coefficients

Sample Size	Metric Quality of Criterion					
	Dichotomous			Polychotomous (5)		
	OLS	Ridge	Jackknife	OLS	Ridge	Jackknife
25	.034	.140	.034	.007	.117	.007
50	.034	.159	.034	.007	.132	.007
100	.034	.171	.034	.007	.145	.007

TABLE 5

Mean Standard Error of Coefficients

Sample Size	Metric Quality of Criterion					
	Dichotomous			Polychotomous (5)		
	OLS	Ridge	Jackknife	OLS	Ridge	Jackknife
25	.309	.052	.351	.239	.054	.271
50	.204	.023	.214	.157	.027	.131
100	.140	.012	.142	.107	.017	.109

TABLE 6

Mean t-Statistic for Coefficients

Sample Size	Metric Quality of Criterion					
	Dichotomous			Polychotomous (5)		
	OLS	Ridge	Jackknife	OLS	Ridge	Jackknife
25	.736	1.802	.702	1.081	2.148	1.030
50	1.086	2.997	1.105	1.594	3.481	1.631
100	1.561	4.577	1.647	2.308	5.234	2.389

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56 Hillhouse Avenue
New Haven, CT 06520

Dr. Asa G. Hilliard, Jr.
The Urban Institute for
Human Services, Inc.
P.O. Box 15068
San Francisco, CA 94115

Dr. Charles L. Hulin
Department of Psychology
University of Illinois
Champaign, IL 61820

Dr. Rudi Klauss
Syracuse University
Public Administration Department
Maxwell School
Syracuse, NY 13210

Dr. Judi Komaki
Georgia Institute of Technology
Engineering Experiment Station
Atlanta, GA 30332

Dr. Arthur L. Korotkin
Vice-President and Director
Washington Office
Richard A. Gibbone Associates, Inc.
10605 Concord St., Suite 203A
Kensington, MD 20795

Dr. Edward E. Lawler
Battelle Human Affairs Research
Centers
4000 N.E. 41st Street
P.O. Box 5395
Seattle, WA 98105

LIST 4 (continued)

Dr. Arie Y. Lewin
Duke University
Duke Station
Durham, NC 27706

Dr. Ernest R. May
Harvard University
John Fitzgerald Kennedy
School of Government
Cambridge, MA 02138

Dr. Arthur Stone
State University of New York
at Stony Brook
Department of Psychology
Stony Brook, NY 11794

Dr. D. M. Nebeker
Navy Personnel R&D Center
San Diego, CA 92152

Dr. Thomas M. Ostrom
The Ohio State University
Department of Psychology
116E Stadium
404C West 17th Avenue
Columbus, OH 43210

Dr. Manuel Ramierz
University of California at Santa Cruz
Clark Kerr Hall #25
Santa Cruz, CA 95064

Dr. Saul B. Sells
Institute of Behavioral Research
Drawer C
Texas Christian University
Fort Worth, TX 76129

Dr. Richard Steers
Graduate School of Management
and Business
University of Oregon
Eugene, OR 97403

Dr. James R. Terborg
University of Houston
Department of Psychology
Houston, TX 77004

Dr. Howard M. Weiss
Purdue University
Department of Psychological Sciences
West Lafayette, IN 47907

Dr. Philip G. Zimbardo
Stanford University
Department of Psychology
Stanford, CA 94305

Dr. Joseph Olmstead
Human Resources Research Organization
300 North Washington Street
Alexandria, VA 22314

Dr. Edwin Locke
University of Maryland
College of Business and Management
and Department of Psychology
College Park, MD 20742

Dr. Clayton P. Alderfer
Yale University
School of Organization and Management
New Haven, CT 06520

Dr. Larry Cummings
University of Wisconsin-Madison
Graduate School of Business
Center for the Study of
Organizational Performance
1155 Observatory Drive
Madison, WI 53706

Dr. Benjamin Schneider
University of Maryland
Department of Psychology
College Park, MD 20742

LIST 5

MISCELLANEOUS

Air Force

AFOSR/NL (Dr. Fregly)
Building 410
Bolling AFB
Washington, DC 20332

Military Assistant for Human Resources
OAD (E&LS) ODDR&E
Pentagon 3D129
Washington, DC 20301

Technical Director
AFHRL/ORS
Brooks AFB, TX 78235

AFMPC/DPMYP
(Research and Measurement Division)
Randolph AFB, TX 78148

Air University Library/LSE 76-443
Maxwell AFB, AL 36112

Air Force Institute of Technology
AFIT/LSGR (Lt. Col. Umstot)
Wright-Patterson AFB, OH 45433

Army

Office of the Deputy Chief of Staff
for Personnel, Research Office
ATTN: DAPE-PBR
Washington, DC 20310

Army Research Institute (2 copies)
5001 Eisenhower Avenue
Alexandria, VA 22333

ARI Field Unit - Leavenworth
P.O. Box 3122
Fort Leavenworth, KS 66027

Headquarters FORSCOM
ATTN: AFPR-HR
Ft. McPherson, GA 30330

CAPT Joseph Weker
Department of the Army
Headquarters, 32D Army Air
Defense Command
APO New York 09175

ARI Field Unit - Monterey
P.O. Box 4787
Monterey, CA 93940

Marine Corps

Dr. A. L. Slafkosky
Code RD-1
HQ U.S. Marine Corps
Washington, DC 20380

Commandant of the Marine Corps
(Code MPI-20)
Washington, DC 20380

Coast Guard

Mr. Richard Lanterman
Chief, Psychological Research Branch
U.S. Coast Guard (G-P-1/2/62)
Washington, DC 20590

Navy

Office of the DCNO(MPT)
Scientific Advisor (OP-01T)
Washington, DC 20350

Office of the DCNO(MPT)
OP-15
Director, Human Resource Management
Division
Washington, DC 20372

CAPT Paul D. Nelson, MSC, USN
Director of Manpower & Facilities
(Code 60)
5105 Building 5 PTX
Washington, DC 20372

LIST 5 (continued)

Office of the Commanding Officer
Navy Medical R&D Command
Bethesda, MD 20014

Superintendent (Code 1424)
Naval Postgraduate School
Monterey, CA 93940

Office of the DCNO
Head, R, D, and S Branch (OP-102)
Washington, DC 20350

Office of the DCNO
Director, HRM Plans and Policy Branch
OP-150
Washington, DC 20350

Professor John Senger
Operations Research & Admin. Science
Naval Postgraduate School
Monterey, CA 93940

Training Officer
Human Resource Management Center
Naval Training Center (Code 9000)
San Diego, CA 92133

Scientific Director
Naval Health Research Center
San Diego, CA 92152

Commanding Officer
Naval Submarine Medical Research Lab.
Naval Submarine Base
New London, Box 900
Groton, CT 06340

Commanding Officer
Naval Training Equipment Center
Technical Library
Orlando, FL 32813

NAMRL, NAS
Pensacola, FL 32508

Chief of Naval Technical Training
Code 0161
NAS Memphis (75)
Millington, TN 38054

Human Resource Management Detachment
Naples
Box 3
FPO New York 09521

Navy Military Personnel Command (2 copies)
HRM Department (NMPC-6)
Washington, DC 20350

Human Resource Management Detachment
Rota
Box 41
FPO New York 09540

Human Resource Management Center
Norfolk
5621-23 Tidewater Drive
Norfolk, VA 23511

Human Resource Management Center
Building 304
Naval Training Center
San Diego, CA 92133

Office of Naval Research (Code 200)
Arlington, VA 22217

ACOS Research & Program Development
Chief of Naval Education & Training (N-5)
Naval Air Station
Pensacola, FL 32508

Human Resource Management School
Naval Air Station Memphis (96)
Millington, TN 38054

Director, Human Resource Training Dept.
Naval Amphibious School
Little Creek
Naval Amphibious Base
Norfolk, VA 23521

LIST 5 (continued)

Naval Material Command
Management Training Center (NMAT 09M32)
Room 150 Jefferson Plaza, Bldg. #2
1421 Jefferson Davis Highway
Arlington, VA 20360

Commanding Officer
HRMC Washington
1300 Wilson Blvd.
Arlington, VA 22209

Head, Research and Analysis Branch
Navy Recruiting Command (Code 434)
801 North Randolph Street, Room 8001
Arlington, VA 22203

LCDR William Maynard
Psychology Department
National Naval Medical Center
Bethesda, MD 20014

CAPT Donald F. Parker, USN
Command Officer
Navy Personnel R&D Center
San Diego, CA 92152

Dr. Myron M. Zajkowski
Senior Scientist
Naval Training Analysis and
Evaluation Group
Orlando, FL 32813

Other

Organizational Psychology Research Group
Office of Personnel Management
1900 E. Street, N.W.
Washington, D.C. 20415

HumRRO (Attn: Library)
300 North Washington Street
Alexandria, VA 22314

Office of the Air Attache (S3B)
Embassy of Australia
1601 Massachusetts Avenue, N.W.
Washington, DC 20036

Scientific Information Officer
British Embassy - Room 509
3100 Massachusetts Avenue, N.W.
Washington, DC 20008

Canadian Defense Liaison Staff,
Washington
2450 Massachusetts Avenue, N.W.
Washington, DC 20008
ATTN: CORD

Mr. Luigi Petrullo
2431 North Edgewood Street
Arlington, VA 22207

Dr. Eugene F. Stone
Assistant Professor of Administrative
Sciences
Krannert Graduate School
Purdue University
West Lafayette, IN 47907

Mr. Mark T. Munger
McBer and Company
137 Newbury Street
Boston, MA 02116

Commandant
Royal Military College of Canada
Kingston, Ontario
K7L 2W3
ATTN: Department of Military
Leadership and Management

Dr. Richard T. Mowday
Graduate School of Management
and Business
University of Oregon
Eugene, OR 97403

National Defense Headquarters
Ottawa, Ontario
K1A 0K2
ATTN: DPAR

LIST 5 (continued)

CDR William A. Earner
Management Department
Naval War College
Newport, RI 02940

Mr. Martin Milrod
Educational Equity Grants Program
1200 19th Street, N.W.
National Institute of Education
Washington, DC 20208

CAPT Richard L. Martin, USN
Commanding Officer
USS Francis Marion (LPA-249)
FPO New York 09501

ATTN: Library
ARI Field Unit - USAREUR
c/o DCSPER
APO New York 09403

MAJ Robert Miltrout
Mr. Richard Grann
U.S. Army Trimis-Evaluation Unit
Walter Reed Army Medical Center
Washington, D.C. 20012

Mr. Thomas N. Martin
Department of Administrative Sciences
College of Business and Administration
Southern Illinois University
Carbondale, IL 62901